

Modeling and Simulation of Droplet Dynamics with Species Discontinuity at the Interface

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Understanding the complex interaction of droplet dynamics with mass transfer and chemical reactions is of fundamental importance in liquid-liquid extraction. High-fidelity numerical simulation of droplet dynamics with interfacial mass transfer is particularly challenging because the position of the interface between the fluids and the interface physics must be predicted as part of the solution of the flow equations. In this work, we propose a global embedded interface formulation to model the jump in species concentration at an interface in thermodynamic equilibrium. The formulation is implemented and tested in a volume-tracking fluid-flow solver. Simulations of single droplet with different distribution coefficients are performed in 3D to demonstrate the new capability.

Droplets dynamics with mass transfer is encountered in several industrial processes, as for example in liquid-liquid extraction, where the extraction process takes place at the liquid-liquid interface. High-fidelity simulation of droplet dynamics can play an important role in our understanding of the underlying physics, in particular the interphase mass transfer process. Furthermore, the simulation results can be used to derive constitutive equations for droplet size and velocity distributions for the multiphase flow formulation, helping to reduce the uncertainties of current models, which are empirical and/or based on simplistic assumptions.

Our goal is to develop accurate computational capabilities to simulate droplets dynamics relevant to liquid-liquid extraction. Achieving high-fidelity simulation of droplets dynamics with interfacial mass transfer is very challenging because the interface between the fluids must be predicted as part of the solution of the Navier-Stokes flow equations. In addition, surface tension and the discontinuity in fluid

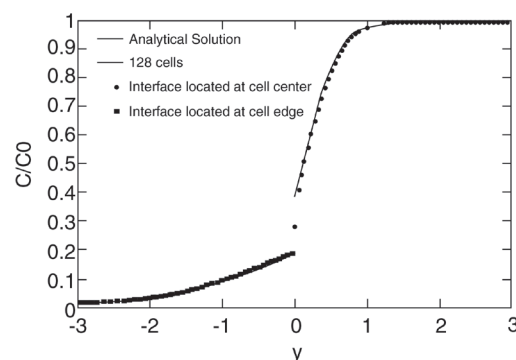
density, viscosity, and species concentration at the interface present additional numerical challenges. We have recently proposed a global embedded interface formulation to model the interfacial conditions of an interface in thermodynamic equilibrium [1], which we have implemented and tested within the balanced-force volume-tracking algorithm of Francois et al. [2]. In the volume-tracking method, a single-field formulation for the governing flow equations is employed (single velocity, single pressure), the multiple fluids are represented by their volume

fraction (amount of fluid in a computational cell), and the interface is reconstructed piecewise by linear plane from the volume fraction information. The interface is therefore embedded within the computational mesh. The formulation is presented in detail in [1].

The global embedded interface formulation consists of deriving an equivalent model for the species transport equation and the interfacial boundary conditions. The species transport equation is an advection-diffusion equation, with continuity of the solute flux across the interface—at thermodynamic equilibrium, the species concentration on both sides of the interface can be discontinuous ($C_2/C_1=m$, with m known as the distribution coefficient). It is this discontinuity in species concentration at the interface that is numerically challenging. To circumvent this difficulty, we have derived an equivalent model that embeds the interface conditions implicitly within the solution by introducing a change in variable.

To verify the species-transport solver and our global embedded interface model, we consider the diffusion of a single species in a system of two fluids separated by an interface in 1D. Initially, the concentration is constant—equal to C_0 in fluid 1 and zero in fluid 2. The analytical solution for an infinite domain with the interface located at zero is given in Crank [3]. For our computations, we consider a domain size $[-1.5, 1.5]$ and a case with a distribution coefficient of $m=5$, a diffusion ratio of $D_2/D_1=1$, and 128 cells. The species concentration profile is plotted in Fig. 1 at time $t=0.1$, along with the analytical solution. Our computations capture the jump in the species concentration values and are in very good agreement with the analytical solution. If the

Fig. 1. One-dimensional species diffusion verification test case for the global embedded interface formulation. The interface between fluid 1 and fluid 2 is located in the center of the domain (at $y=0$). The distribution coefficient is $m=0.5$ and diffusion coefficient ratio is $D_2/D_1=10$. The results are shown at time $t=0.1$ using 128 computational cells.



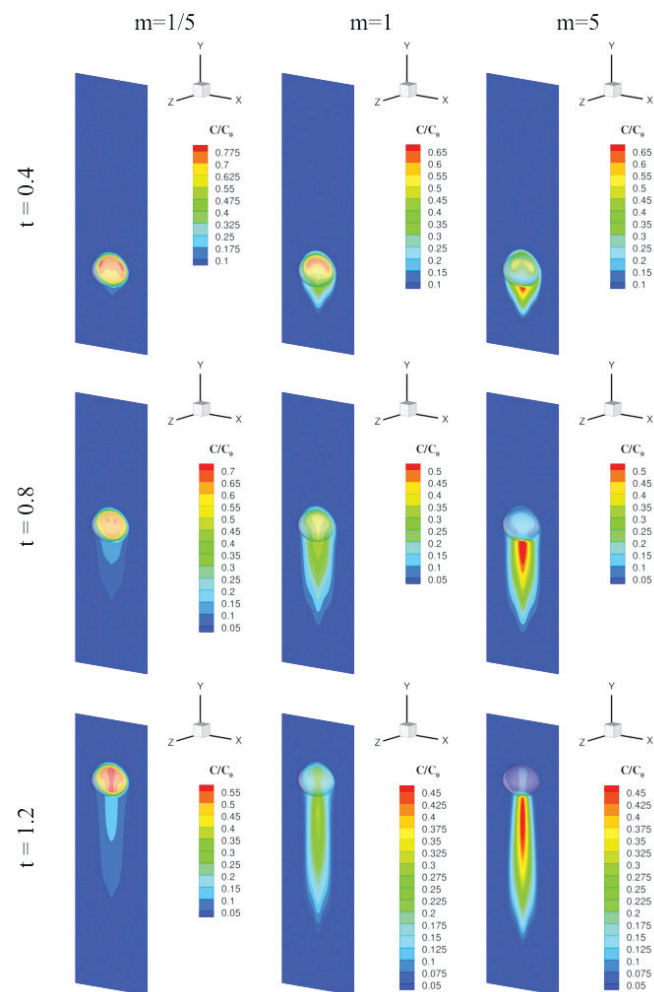


Fig. 2. Droplet shape and species concentration contours for 3D droplet rising by buoyancy. The Weber number is 0.22, the Peclet number is 1600 and the Reynolds number is 8. The results are shown at time $t=0.4$, 0.8 , and 1.2 with $m=1/5$, 1 , and 5 . The mesh size is $40 \times 40 \times 120$. The surface tension coefficient is constant. The Reynolds number represents the ratio between inertia and viscous force, the Weber number represents the ratio between inertia and surface tension, and the Peclet number represents the ratio between advection and diffusion.

interface is located on a cell edge (i.e., the volume fraction in the cell just left of the interface is 1 and in the cell just right of the interface the volume fraction is 0), the discontinuity is captured accurately and is sharp. If the interface is located within a computational cell (i.e., the volume fraction is between 0 and 1), the results show an intermediate value, that is, the discontinuity is spread over one cell.

To demonstrate our droplet dynamics simulation capability, we have performed simulations of a single droplet rising by buoyancy in 3D for different m . Initially, the droplet concentration is unity and the background fluid concentration is zero. The droplet shapes and species concentration contours are shown in Fig. 2 at different times, and the droplet velocity and droplet concentration are plotted versus time in Fig. 3. From the droplet velocity one can derive the drag coefficient, and from the species concentration one can derive the mass transfer coefficient. As expected for this low Reynolds number case, the droplet rises and deforms to an ellipsoidal shape. The species concentration distribution in the droplet and behind the droplet is different for the three distribution coefficients. Species transport faster from the

droplet to the background fluid and have a higher concentration at the trailing edge of the droplet for the case $m=5$. In contrast, the species concentration dissipates more slowly and with a shorter trace for the case of $m=1/5$ (red in Fig. 2). For the case with the larger distribution coefficient ($m=5$), the droplet loses its species concentration the fastest. The distribution coefficient has no effect on the droplet velocity since the surface tension here is a constant, so there is no soluto-capillary effect (the effect of the concentration is not back-coupled to the fluid flow). Note that these simulations are preliminary as they were performed on a rather coarse mesh. Future work will include simulation on finer meshes and simulations of multiple droplets.

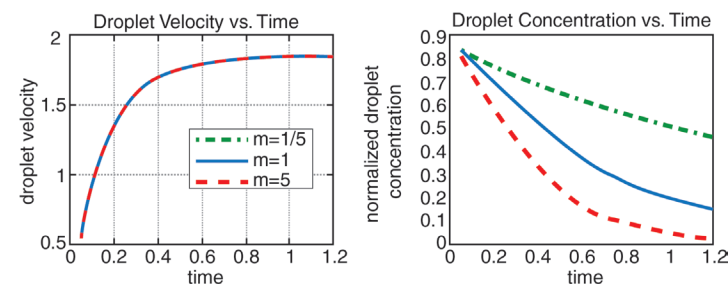


Fig. 3. Effects of the distribution coefficient (m) on (a) droplet velocity, and (b) droplet concentration. The Reynolds number is 8, the Weber number is 0.22, and the Peclet number is 1600. The surface tension coefficient is constant.

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